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A Cauchy–Khinchin matrix inequality

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Abstract

We derive a matrix inequality, which generalizes the Cauchy–Schwarz inequality for vectors, and Khinchin's inequality for zero–one matrices. Furthermore, we pose a related problem on the maximum irregularity of a directed graph with prescribed number of vertices and arcs, and make some remarks on this problem. © 1998 Elsevier Science Inc. All rights reserved.

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1. Introduction

In a recent paper, de Caen [1] presented an upper bound on the sum of squares of degrees in a graph. His result was obtained by considering some positive semidefinite quadratic form related to the line graph of the complete graph. In this paper we exploit this idea, which can be applied more generally, to obtain an inequality on arbitrary real matrices, and which generalizes Cauchy's inequality for vectors. Surprisingly, the matrix inequality can also be derived by applying Cauchy's inequality to a special vector related to the matrix. When we apply our result to zero–one matrices it reduces to a minor (and already known, cf. [2]) improvement of Khinchin's inequality [3] for such matrices. Khinchin [4] applied his result to prove a surprising number theoretic result.

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We also generalize our result to a “Cauchy–Schwarz matrix inequality”, which looks a bit complicated, but nevertheless may have some useful applications. When we apply it to a square matrix and its transpose, we obtain another interesting matrix inequality, which resembles a Khinchin-type inequality for zero–one matrices found by Matúš (cf. [2]). This resemblance pointed us to a problem on directed graphs (note that zero–one matrices can be identified with directed graphs). We wish to maximize some quantity which measures the irregularity of the graph, over all directed graphs with a prescribed number of vertices and arcs. A similar problem has been studied by several authors (cf. [5–7]), and turned out to have a rather complicated solution. In the final section of this paper we make some remarks on the new problem.

2. The matrix inequality

Theorem 1. *Let X be a real $m \times n$ matrix. Then*

$$\left(\sum_{i=1}^m \sum_{j=1}^n X_{ij} \right)^2 + mn \sum_{i=1}^m \sum_{j=1}^n X_{ij}^2 \geq m \sum_{i=1}^m \left(\sum_{j=1}^n X_{ij} \right)^2 + n \sum_{j=1}^n \left(\sum_{i=1}^m X_{ij} \right)^2$$

with equality if and only if $X_{ij} = y_i + z_j$ for some real vectors y and z , and all i and j .

Proof. To derive the inequality, we associate it with a quadratic form in mn variables. To do this we need to introduce some $mn \times mn$ matrices, with rows and columns indexed (symmetrically) by the ordered pairs (i, j) , $i = 1, \dots, m$, $j = 1, \dots, n$. Let A_1 denote the $(0, 1)$ -matrix which is 1 in the entry $((i, j), (i', j'))$ if and only if $i = i'$. Similarly let A_2 denote the $(0, 1)$ -matrix which is 1 in the entry $((i, j), (i', j'))$ if and only if $j = j'$. Now possibly after rearranging the indices we have that $A_1 = I_m \otimes J_n$ and $A_2 = J_m \otimes I_n$, where I and J are identity and (square) all-ones matrices, respectively, with indices denoting the sizes, and \otimes denotes the Kronecker product. Now one easily checks that the inequality is equivalent to

$$X^T(J_{mn} + mnI_{mn} - mI_m \otimes J_n - nJ_m \otimes I_n)X \geq 0,$$

where X is regarded as a column vector of size mn . So the inequality is proven if we can show that $R = J_{mn} + mnI_{mn} - mI_m \otimes J_n - nJ_m \otimes I_n$ is positive semidefinite. To show this, we note that the four matrices J_{mn} , I_{mn} , $I_m \otimes J_n$ and $J_m \otimes I_n$ mutually commute. Hence they have a common basis of eigenvectors, and we can thus find the eigenvalues of R by combining the eigenvalues of its summands on each common eigenspace, as is done in the following table. This shows that R has eigenvalues 0 and mn , so indeed it is positive semidefinite.

J_{mn}	I_{mn}	$I_m \otimes J_n$	$J_m \otimes I_n$	R	(multiplicity)
mn	1	n	m	0	(1)
0	1	n	0	0	$(m-1)$
0	1	0	m	0	$(n-1)$
0	1	0	0	mn	$((m-1)(n-1))$

Moreover, we have equality in the bound if and only if X is an eigenvector of R with eigenvalue 0 (for convenience we also consider the zero vector as an eigenvector). From the above table, it follows that this is the case if and only if $X = Y + Z$, for some eigenvector Y of $I_m \otimes J_n$ with eigenvalue n , and some eigenvector Z of $J_m \otimes I_n$ with eigenvalue m . But this means precisely that for fixed i , Y_{ij} is constant, i.e. $Y_{ij} = y_i$ for some vector y , and similarly $Z_{ij} = z_j$ for some vector z . \square

Theorem 1 is proven in a similar fashion as de Caen's inequality [1] (see below). His result was obtained by considering some positive semidefinite matrix in the Bose–Mesner algebra of the triangular 2-class association scheme, while here we consider one in the Bose–Mesner algebra of the rectangular 3-class association scheme. In fact, one can do a similar thing in any association scheme, giving an inequality on a vector X , which is indexed by the vertices of the association scheme. The rectangular scheme seems to be a very natural one, since it gives a matrix inequality. For some background in the theory of association schemes we refer the reader to [8] or [9]. In an arbitrary d -class association scheme on v vertices, with adjacency matrices A_i and dual eigenmatrix Q , we get an inequality by considering a minimal idempotent $E_j = 1/v \sum_{i=0}^d Q_{ij} A_i$. In fact, in this way, and by considering the characteristic vector of a subset of the vertex set, Delsarte [10] (cf. [8]) derived his linear programming bounds on the inner distribution of the subset. Thus for $(0, 1)$ -matrices the matrix inequality (see Section 3) is a direct consequence of Delsarte's linear programming bound.

In a sense, the matrix inequality and de Caen's inequality are equivalent. For example, if $(Z_{\{i,j\}})$ is a real vector indexed by the unordered pairs of a set of size n , then by applying the matrix inequality to the (symmetric) matrix X defined by $X_{ij} = Z_{\{i,j\}}$ if $i \neq j$, and

$$X_{ii} = \frac{2}{n-2} \sum_{j \neq i} Z_{\{i,j\}} - \frac{2}{(n-1)(n-2)} \sum_{\{j,k\}} Z_{\{j,k\}},$$

(after some straightforward, but tedious calculations) we obtain de Caen's inequality

$$\left(\sum_{\{i,j\}} Z_{\{i,j\}}\right)^2 + \binom{n-1}{2} \sum_{\{i,j\}} Z_{\{i,j\}}^2 \geq \frac{n-1}{2} \sum_i \left(\sum_{j \neq i} Z_{\{i,j\}}\right)^2.$$

Going back from this inequality to the matrix inequality is also possible, but we shall not do that here.

Also Cauchy's famous inequality can be derived: let x be a real vector of size m , then by applying the matrix inequality to the $m \times 2$ matrix $[x \ -x]$, we find that $(\sum_{i=1}^m x_i)^2 \leq m \sum_{i=1}^m x_i^2$. Note that Cauchy's inequality also follows from considering the positive semidefinite matrix $mI_m - J_m$ (in the Bose–Mesner algebra of the complete 1-class association scheme, or in fact, any association scheme). Surprisingly, we can also find the matrix inequality (and hence give another proof of it) by applying Cauchy's inequality, i.e., to the vector $(X_{ij} - (1/n)r_i - (1/m)c_j)_{ij}$ indexed by the mn ordered pairs, where $r_i = \sum_{k=1}^n X_{ik}$ is the i th row sum of X and $c_j = \sum_{k=1}^m X_{kj}$ is the j th column sum of X . As Cauchy's inequality is a special case of the Cauchy–Schwarz inequality $|\langle x, y \rangle| \leq \|x\| \|y\|$ (or its slightly improved version $(m\langle x, y \rangle - \sum_{i=1}^m x_i \sum_{i=1}^m y_i)^2 \leq (m\|x\|^2 - (\sum_{i=1}^m x_i)^2)(m\|y\|^2 - (\sum_{i=1}^m y_i)^2)$), this calls for the following generalization of Theorem 1.

Theorem 2. Let X and Y be real $m \times n$ matrices with row sums r_i and r'_i , column sums c_j and c'_j , and entries summing to σ and σ' , respectively. Then

$$\begin{aligned} & \left(\sigma\sigma' + mn \sum_{i=1}^m \sum_{j=1}^n X_{ij}Y_{ij} - m \sum_{i=1}^m r_i r'_i - n \sum_{j=1}^n c_j c'_j \right)^2 \\ & \leq \left(\sigma^2 + mn \sum_{i=1}^m \sum_{j=1}^n X_{ij}^2 - m \sum_{i=1}^m r_i^2 - n \sum_{j=1}^n c_j^2 \right) \\ & \quad \cdot \left(\sigma'^2 + mn \sum_{i=1}^m \sum_{j=1}^n Y_{ij}^2 - m \sum_{i=1}^m r_i'^2 - n \sum_{j=1}^n c_j'^2 \right). \end{aligned}$$

Proof. Consider the positive semidefinite matrix R from the proof of Theorem 1 and, again, consider X and Y as vectors. Now also the 2×2 matrix

$$\begin{pmatrix} X^T R X & X^T R Y \\ Y^T R X & Y^T R Y \end{pmatrix} = \begin{pmatrix} X^T \\ Y^T \end{pmatrix} R (X \ Y)$$

is positive semidefinite. Hence it has a nonnegative determinant, and the result follows. \square

Again surprisingly, Theorem 2 is in itself a generalization of the Cauchy–Schwarz inequality. For vectors x and y we obtain Cauchy–Schwarz by applying Theorem 2 to the matrices $[x \ -x]$ and $[y \ -y]$.

In case we have a square matrix X we can apply the result to X and its transpose X^T to obtain the following.

Corollary 1. *Let X be a real $n \times n$ matrix with row sums r_i and column sums c_j . Then*

$$\sum_{i=1}^n (r_i - c_i)^2 \leq n \sum_{i=1}^n \sum_{j=1}^n X_{ij}^2 - n \sum_{i=1}^n \sum_{j=1}^n X_{ij} X_{ji} = n \operatorname{Trace}(XX^T - X^2).$$

Proof. Theorem 2 applied to X and X^T reduces to $\sigma^2 + n^2 \sum_{i=1}^n \sum_{j=1}^n X_{ij} X_{ji} - 2n \sum_{i=1}^n r_i c_i \leq \sigma^2 + n^2 \sum_{i=1}^n \sum_{j=1}^n X_{ij}^2 - n \sum_{i=1}^n r_i^2 - n \sum_{j=1}^n c_j^2$, since the right-hand side is nonnegative, and the inequality follows. Now note that for any two $n \times n$ matrices A and B we have that $\sum_{i=1}^n \sum_{j=1}^n A_{ij} B_{ij} = \sum_{i=1}^n (AB^T)_{ii} = \operatorname{Trace}(AB^T)$. \square

3. Khinchin-type inequalities for zero-one matrices

In the special case of $(0, 1)$ -matrices, the inequality of Theorem 1 reduces to the following Khinchin-type inequality. It was found earlier by Matúš and Tuzar [2], however by using different methods (from measure theory).

Proposition 1. *Let X be an $m \times n$ $(0, 1)$ -matrix, with row sums r_i , column sums c_j , and entries summing to σ . Then*

$$m \sum_{i=1}^m r_i^2 + n \sum_{j=1}^n c_j^2 \leq \sigma^2 + mn\sigma,$$

with equality if and only if X has constant rows (i.e., only rows of all-ones and rows of all-zeroes) or constant columns.

Proof. The inequality is an obvious consequence of Theorem 1. In case of equality $X_{ij} = y_i + z_j$ for some y and z . Now suppose X has a row that is not constant, say $X_{ij} = 0$ and $X_{ih} = 1$. From this we get that $z_h = z_j + 1$, which implies that for any row k we have that $X_{kh} = y_k + z_h = y_k + z_j + 1 = X_{kj} + 1$, and hence $X_{kj} = 0$ and $X_{kh} = 1$. This proves that X has constant columns. Thus, in case of equality we have constant rows or constant columns. On the other hand, it is also clear that if X has constant rows or constant columns, then we indeed have equality. \square

This inequality is an improvement (in the nonsquare case) of a result by Khinchin [3], who proved that $l \sum_{i=1}^m r_i^2 + l \sum_{j=1}^n c_j^2 \leq \sigma^2 + l^2 \sigma$, where $l = \max\{m, n\}$. Khinchin [4] applied his inequality to prove a surprising number

theoretic result. He showed that the set of integer squares S is a so-called essential component, that is, for any proper subset A of the positive integers,

$$\inf_{n=1,2,\dots} \frac{|(S+A)_n|}{n} > \inf_{n=1,2,\dots} \frac{|A_n|}{n},$$

where $B_n = \{x \in B \mid x \leq n\}$ for a set B . Note that $\inf \{|S_n|/n \mid n = 1, 2, \dots\} = 0$.

Several optimization problems concerning $(0, 1)$ -matrices have been studied, a particular one being the problem of optimizing $\sum_{i=1}^n r_i c_i$ for a square matrix of given size and given number σ of entries which are equal to one (cf. [1, 5–7]). Note that for a symmetric matrix with zero diagonal this is the problem of optimizing the sum of squares of degrees in an undirected graph. Also several inequalities for $(0, 1)$ -matrices have been derived, in particular, Matúš (cf. [2]) found that $\sum_{i=1}^n (r_i - c_i)^2 \leq n\sigma - \sum_{i=1}^n r_i c_i$. This inequality strongly resembles the inequality of Corollary 1, however, the two are incomparable. Here the problem arises of maximizing $\sum_{i=1}^n (r_i - c_i)^2$, given n and σ . In Section 4 we shall make some remarks concerning this directed graph problem.

4. A problem on directed graphs

A square $(0, 1)$ -matrix X is the same as a directed graph G without multiple arcs (but allowing loops and digons). (For some background in directed graphs we refer the reader to [11].) From u to v there is an arc (u, v) if and only if $X_{uv} = 1$. It is then clear that a vertex u has outdegree $d_u^+ = r_u$, the u th row sum of X , and in-degree $d_u^- = c_u$, the u th column sum of X . Our $(0, 1)$ -matrix problem is now formulated as a directed graph problem: maximize $\sum_{u \in V} (d_u^+ - d_u^-)^2$, where V denotes the vertex set of G , over all graphs G with given number n of vertices and given number σ of arcs. From a graph-theoretic point, the quantity that we are maximizing measures the irregularity of the digraph, and hence is of interest.

Let $G(n, \sigma)$ denote the set of all directed graphs without multiple arcs, with n vertices and σ arcs, and let $\sigma_2(G)$ denote $\sum_{u \in V} (d_u^+ - d_u^-)^2$ in a given graph G . Furthermore, define $f(n, \sigma) = \max\{\sigma_2(G) \mid G \in G(n, \sigma)\}$. Note that $f(n, \sigma) \leq n\sigma$ by Corollary 1. We shall see later that equality holds if and only if there is a directed complete bipartite graph in $G(n, \sigma)$. We shall also show that $f(n, \sigma) \leq \frac{1}{3}(n^3 - n)$, and characterize the case of equality. Note that the inequality also follows from Matúš inequality $\sum_{u \in V} (d_u^+ - d_u^-)^2 \leq n\sigma - \sum_{u \in V} d_u^+ d_u^-$ and the inequality $\sum_{u \in V} d_u^+ d_u^- \geq n\sigma - \frac{1}{3}(n^3 - n)$ (cf. [12]). Note also that if a graph minimizes $\sum_{u \in V} d_u^+ d_u^-$ and has equality in Matúš inequality, then it also maximizes $\sum_{u \in V} (d_u^+ - d_u^-)^2$, and solves our problem. This is for example the case if $\sigma = \binom{n}{2} - \frac{1}{2}n$, when a graph minimizing $\sum_{u \in V} d_u^+ d_u^-$ must be a directed transitive complete multipartite graph $K_{2,\dots,2}$ (that is, the graph obtained by taking the undirected version, and directing all edges in the same direction) (cf.

[6]). The complete solution to the problem of minimizing $\sum_{u \in V} d_u^+ d_u^-$ is supposed to be in [7], however, not all minimizing graphs are characterized there (for example, the directed transitive complete multipartite graphs $K_{1,2,3}$ and $K_{1,3,2}$ are not mentioned as solutions in $G(6, 11)$). Therefore, we shall not use these results. Besides that, many solutions do not have equality in Matúš' inequality, and hence we have to do some work ourselves anyway.

Lemma 1. *If G is a graph maximizing $\sigma_2(G)$ over all graphs in $G(n, \sigma)$ such that for some vertices u and v neither (u, v) nor (v, u) is an arc in G , then G does not have digons or loops.*

Proof. Suppose G has a loop at some vertex, say w (which may be u or v), and suppose without loss of generality that $d_u^+ - d_u^- \geq d_v^+ - d_v^-$. Now consider the graph $G' \in G(n, \sigma)$ which is obtained from G by replacing the arc (w, w) (the loop at w) by the arc (u, v) . Then

$$\begin{aligned}\sigma_2(G') &= (d_u^+ - d_u^- + 1)^2 + (d_v^+ - d_v^- - 1)^2 + \sum_{z \neq u, v} (d_z^+ - d_z^-)^2 \\ &= \sigma_2(G) + 2(d_u^+ - d_u^-) - 2(d_v^+ - d_v^-) + 2 > \sigma_2(G),\end{aligned}$$

which is a contradiction. Hence G has no loops, and similarly we can prove that G has no digons. \square

This elementary lemma already simplifies the situation substantially, i.e., if $\sigma \leq \binom{n}{2}$, then a maximizing graph will have no loops or digons. If $\sigma > \binom{n}{2}$, then between any two vertices there will be at least one of the possible two arcs.

Note also that $\sigma_2(G) = \sigma_2(\bar{G})$, where \bar{G} is the graph-theoretic complement of G (its adjacency matrix is obtained from that of G by interchanging zeroes and ones). Moreover, if G has σ arcs, then \bar{G} has $n^2 - \sigma$ arcs, hence $f(n, \sigma) = f(n, n^2 - \sigma)$. Without loss of generality we can therefore restrict to the case $\sigma \leq \frac{1}{2}n^2$.

Lemma 2. *If $\binom{n}{2} < \sigma \leq \frac{1}{2}n^2$, then $f(n, \sigma) = f(n, \binom{n}{2})$, and if G is a graph maximizing $\sigma_2(G)$ over all graphs in $G(n, \sigma)$, then between any two distinct vertices in G there will be precisely one arc. If $\sigma \leq \binom{n}{2}$, then a maximizing graph will have no loops or digons.*

Proof. If $\binom{n}{2} < \sigma \leq \frac{1}{2}n^2$, then by the previous lemma there will be at least one arc between any two vertices. Now suppose we have a digon between vertices u and v in the maximizing graph G . It follows from easy counting arguments that there is a vertex, say w , at which there is no loop. If we assume, without loss of generality, that $d_u^+ - d_u^- \geq d_v^+ - d_v^-$, then replacing the arc (v, u) by the loop (w, w) will increase σ_2 , which is a contradiction. Hence G has no digons. Thus

between any two distinct vertices there is precisely one arc, and hence the other arcs are loops. Since adding loops does not change σ_2 , it follows that $f(n, \sigma) = f(n, \binom{n}{2})$. If $\sigma \leq \binom{n}{2}$ then the statement follows immediately from Lemma 1. \square

So now we can restrict to the case $\sigma \leq \binom{n}{2}$, where a maximizing graph will have no digons or loops.

Lemma 3. *If G is a graph maximizing $\sigma_2(G)$ over all graphs in $G(n, \sigma)$, where $\sigma \leq \binom{n}{2}$, and (u, v) is an arc in G , then $d_u^+ - d_u^- \geq d_v^+ - d_v^- + 2$. In particular, G is acyclic.*

Proof. Consider the graph $G' \in G(n, \sigma)$ which is obtained from G by reversing the arc (u, v) . The only vertex degrees changed are those of u and v , so

$$\begin{aligned}\sigma_2(G') &= (d_u^+ - d_u^- - 2)^2 + (d_v^+ - d_v^- + 2)^2 + \sum_{z \neq u, v} (d_z^+ - d_z^-)^2 \\ &= \sigma_2(G) - 4(d_u^+ - d_u^-) + 4(d_v^+ - d_v^-) + 8,\end{aligned}$$

and since $\sigma_2(G') \leq \sigma_2(G)$, the result follows. \square

An obvious generalization of this is that if G is again a graph maximizing $\sigma_2(G)$ over all graphs in $G(n, \sigma)$, then for each vertex u and set $S^+ \subset \Gamma_u^+$ (the set of all vertices v such that (u, v) is an arc), then

$$d_u^+ - d_u^- \geq |S^+| + 1 + \frac{1}{|S^+|} \sum_{v \in S^+} (d_v^+ - d_v^-),$$

and a similar result holds for subsets of Γ_u^- .

Even better, a maximizing graph is not just acyclic, but we can prove that it is transitive, that is, if (u, v) and (v, w) are arcs, then so is (u, w) .

Proposition 2. *If G is a graph maximizing $\sigma_2(G)$ over all graphs in $G(n, \sigma)$, where $\sigma \leq \binom{n}{2}$, then G is transitive.*

Proof. Let (u, v) and (v, w) be arcs in G , and suppose that (u, w) is not. Note that (w, u) cannot be an arc either, since that would contradict the previous lemma. Now let G' be the graph in $G(n, \sigma)$, obtained from G by replacing the arc (v, w) by (u, w) . Then

$$\begin{aligned}\sigma_2(G') &= (d_u^+ - d_u^- + 1)^2 + (d_v^+ - d_v^- - 1)^2 + \sum_{z \neq u, v} (d_z^+ - d_z^-)^2 \\ &= \sigma_2(G) + 2(d_u^+ - d_u^-) - 2(d_v^+ - d_v^-) + 2,\end{aligned}$$

and since $\sigma_2(G') \leq \sigma_2(G)$, it follows that $d_v^+ - d_v^- \geq d_u^+ - d_u^- + 1$. But by the previous lemma, we have that $d_u^+ - d_u^- \geq d_v^+ - d_v^- + 2$, which is a contradiction. \square

In the case $\sigma = \binom{n}{2}$ we have now found the maximizing graph, since up to isomorphism there is only one transitive graph with $\binom{n}{2}$ arcs (a transitive tournament). For such a graph $\sigma_2 = \frac{1}{3}(n^3 - n)$, hence we have found that $f(n, \sigma) = \frac{1}{3}(n^3 - n)$ for $\binom{n}{2} \leq \sigma \leq \frac{1}{2}n^2$. Moreover, it is easy to show that for $\sigma < \binom{n}{2}$ we have that $f(n, \sigma + 1) \geq f(n, \sigma) + 2$, hence $f(n, \sigma) < \frac{1}{3}(n^3 - n)$ for $\sigma < \binom{n}{2}$. In these cases the obtained necessary conditions still do not characterize the maximizing graphs, as we can see from the graph with arc set $\{(1, 2), (1, 3), (1, 4), (2, 4)\}$ in $G(4, 4)$. Note that the maximizing graph here is the directed complete bipartite one (that is, the graph with arc set $\{(1, 3), (1, 4), (2, 3), (2, 4)\}$). In fact, any directed complete bipartite graph $K_{a, n-a}$ is a maximizing graph in $G(n, a(n-a))$. Even better, we can apply Theorem 1 to the skew-symmetric $(0, \pm 1)$ -adjacency matrix X of a graph G without loops and digons (i.e., $X_{uv} = -X_{vu} = 1$ if (u, v) is an arc) to find that $\sigma_2(G) \leq n\sigma$ with equality if and only if G is directed complete bipartite (or empty). However, it is not true in general that a maximizing graph in $G(n, \sigma)$ should be bipartite if $\sigma \leq \frac{1}{4}n^2$ (that is, if $G(n, \sigma)$ contains a bipartite graph). Note that this is the case in the problem of minimizing $\sum_{u \in V} d_u^+ d_u^-$ (cf. [6]). We suspect that the general solution to our problem will be as complicated as that minimization problem.

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